

# Surface Effects in the Unitary Fermi Gas

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## Abstract

We study the extended Thomas-Fermi (ETF) density functional of the superfluid unitary Fermi gas. This functional includes a gradient term which is essential to describe accurately the surface effects of the system, in particular with a small number of atoms, where the Thomas-Fermi (local density) approximation fails. We find that our ETF functional gives density profiles which are in good agreement with recent Monte Carlo results and also with a more sophisticated superfluid density functional based on Bogoliubov-de Gennes equations. In addition, by using extended hydrodynamics equations of superfluids, we calculate the frequencies of collective surface oscillations of the unitary Fermi gas, showing that quadrupole and octupole modes strongly depend on the number of trapped atoms.

## I. INTRODUCTION

In a system of spin 1/2 interacting fermions, the unitary regime is commonly referred to as the situation in which the s-wave scattering length  $a$  greatly exceeds the average interparticle separation, thus  $n|a|^3 \gg 1$ , where  $n$  is the number density [1]. In 2002 it was shown experimentally that such systems are (meta)stable [2], and they have been studied extensively ever since [1]. On the basis of very accurate Monte Carlo results, we have recently introduced a simple but reliable extended Thomas-Fermi (ETF) density functional for the unitary Fermi gas at zero temperature [3].

In this paper we show new results obtained with our ETF functional. In particular, we analyze the density profiles of the balanced zero-temperature unitary Fermi gas confined by a harmonic trap, finding that our ETF functional gives density profiles which are in good agreement with recent Monte Carlo results [4,5] and with a more sophisticated superfluid density functional based on Bogoliubov-de Gennes equations [6]. We then obtain extended hydrodynamics equations of superfluids by considering small, time-dependent perturbations of the ETF functional around its ground-state. We show that, under isotropic harmonic confinement, the quadrupole and octupole frequencies of a Fermi gas at unitarity depend on the number of confined atoms, contrary to the monopole and dipole frequencies, which are solely determined by the external potential.

## II. EXTENDED THOMAS-FERMI DENSITY FUNCTIONAL

At zero temperature the Thomas-Fermi (TF) energy functional [1] of a dilute and ultra-cold unpolarized two-component Fermi gas trapped by an external potential  $U(\mathbf{r})$  is

$$E_{TF} = \int d^3\mathbf{r} \, n(\mathbf{r}) [\varepsilon(n(\mathbf{r}); a_F) + U(\mathbf{r})] , \quad (1)$$

with  $\varepsilon(n; a_F)$  bulk energy per particle,  $n(\mathbf{r}) = n_\uparrow(\mathbf{r}) + n_\downarrow(\mathbf{r})$  total density ( $n_\uparrow(\mathbf{r}) = n_\downarrow(\mathbf{r})$ ) and  $a_F$  the s-wave scattering length. The total number of fermions is

$$N = \int d^3\mathbf{r} \, n(\mathbf{r}) . \quad (2)$$

By minimizing  $E_{TF}$  one finds

$$\mu(n(\mathbf{r}); a_F) + U(\mathbf{r}) = \bar{\mu} , \quad (3)$$

with  $\mu(n; a_F) = \frac{\partial(n\varepsilon(n; a_F))}{\partial n}$  bulk chemical potential of a uniform system and  $\bar{\mu}$  chemical potential of the non uniform system.

For the uniform unitary Fermi gas [7] the s-wave scattering length  $a_F$  diverges:

$$a_F \rightarrow \pm\infty , \quad (4)$$

and the only length characterizing the uniform system is the average distance between particles  $n^{-1/3}$ . In this case:

$$\varepsilon(n; \xi) = \xi \frac{3}{5} \frac{\hbar^2}{2m} (3\pi^2)^{2/3} n^{2/3} = \xi \frac{3}{5} \epsilon_F , \quad (5)$$

with  $\epsilon_F$  Fermi energy of the ideal gas and  $\xi$  a universal parameter. The bulk chemical potential associated to Eq. (5) is

$$\mu(n; \xi) = \frac{\partial(n\varepsilon(n))}{\partial n} = \xi \frac{\hbar^2}{2m} (3\pi^2)^{2/3} n^{2/3} = \xi \epsilon_F . \quad (6)$$

The TF functional must be extended to take into account other characteristic lengths related to the spatial variations of the density, besides the average particle separation. As a consequence, the energy per particle must contain additional terms, which scale as the square of the inverse of these various lengths. For this reason, as a simple approximation, we add to the energy per particle the term

$$\lambda \frac{\hbar^2}{8m} \frac{(\nabla n)^2}{n^2} = \lambda \frac{\hbar^2}{2m} \frac{(\nabla \sqrt{n})^2}{n} . \quad (7)$$

Historically, this term was introduced by von Weizsäcker [8] to treat surface effects in nuclei. Moreover, according to the Kirzhnits expansion of the quantum kinetic operator in powers of  $\hbar$  [19],  $\lambda$  must take the value  $\lambda = 1/9$  [19,20] for an ideal, noninteracting, Fermi gas. Here we consider  $\lambda$  as a phenomenological parameter accounting for the increase of kinetic

energy due the spatial variation of the density. We also observe that the TF functional has a pathological behavior at the surface. In fact, the TF density profile becomes zero at a finite distance  $r_{TF}$  from the center of the cloud, while according to quantum mechanics the density must goes to zero only at infinity. This pathology of the TF approximation is efficiently cured by the inclusion of the gradient term (7).

Other recent density-functional methods for unitary Fermi gas have been proposed in the last few years: the Bogoliubov-de Gennes (BdG) superfluid local-density approximation (SLDA) of Bulgac [6] and the Kohn-Sham (KS) density functional approach of Papenbrock [9]. We wish to point out that both the energy functionals proposed by Bulgac [6] and Papenbrock [9] are functionals of the density through single particle orbitals (the BdG or KS orbitals). Therefore they can be used in actual numerical calculations only when the number of fermions is small, since they require a self consistent calculation of single-particle states whose number increases rapidly with the number of particles [17,18]. For completeness, we remark that another density functional for the unitary Fermi gas has been proposed on the basis of the Haldane-Wu statistics [10,11].

Our energy functional, that is the extended Thomas-Fermi (ETF) functional of the unitary Fermi gas, reads

$$E = \int d^3\mathbf{r} \, n(\mathbf{r}) \left[ \lambda \frac{\hbar^2}{8m} \frac{(\nabla n(\mathbf{r}))^2}{n(\mathbf{r})^2} + \xi \frac{3}{5} \frac{\hbar^2}{2m} (3\pi^2)^{2/3} n(\mathbf{r})^{2/3} + U(\mathbf{r}) \right] . \quad (8)$$

We stress that one encounters no severe limitation in the number of particles which may be treated through ETF functionals, since in this case the functional depends only on a single function of the coordinate, i.e. the particle density. By minimizing the ETF energy functional one gets:

$$\left[ -\lambda \frac{\hbar^2}{2m} \nabla^2 + \xi \frac{\hbar^2}{2m} (3\pi^2)^{2/3} n(\mathbf{r})^{2/3} + U(\mathbf{r}) \right] \sqrt{n(\mathbf{r})} = \bar{\mu} \sqrt{n(\mathbf{r})} . \quad (9)$$

This is a sort of stationary 3D nonlinear Schrödinger (3D NLS) equation.

The constants  $\xi$  and  $\lambda$  should be universal i.e. independent on the confining potential  $U(\mathbf{r})$ . The value of the coefficient  $\lambda$  is debated. In the papers of Kim and Zubarev [12]

and Manini and Salasnich [13] the authors set  $\lambda = 1$  over the full BCS-BEC crossover. More recently we have suggested  $\lambda = 1/4$  [14–16]. Note that  $\lambda \simeq 0.25$  was the preliminary prediction at unitarity of effective field theory [21]. We stress, however, that the more recent and accurate prediction of effective field theory based on  $\epsilon$ -expansion is  $\lambda \simeq 0.17$  [22].

### III. FINDING THE UNIVERSAL PARAMETERS OF THE ETF FUNCTIONAL

To determine  $\xi$  and  $\lambda$  we look for the values of the two parameters which lead to the best fit of the ground-state energies obtained by Monte Carlo data for the unitary Fermi gas in a spherical harmonic potential

$$U(\mathbf{r}) = \frac{1}{2}m\omega^2 r^2. \quad (10)$$

We use the more recent and reliable Monte Carlo results with  $N$  even (complete superfluidity): the fixed-node diffusion Monte Carlo (FNDMC) of von Stecher, Greene and Blume [4]. After a systematic analysis [3] we find

$$\xi = 0.455 \quad \text{and} \quad \lambda = 0.13$$

as the best fitting parameters in the unitary regime. The value  $\xi = 0.455$  coincides with that obtained by Perali, Pieri, and Strinati [23] with beyond-mean-field extended BCS theory. Fixing  $\xi = 0.44$  (the Monte Carlo result for a uniform Fermi gas of Carlson *et al.* [24]) we find instead  $\lambda = 0.18$  [3].

In Fig. 1 we plot the ground-state energy  $E$  of the unitary Fermi gas as a function of the number  $N$  of atoms under harmonic confinement of frequency  $\omega$ . In the figure we compare the FNDMC data with even  $N$  [4] with different density functionals: ETF results with best fit ( $\xi = 0.455$  and  $\lambda = 0.13$ ); ETF results obtained from  $\epsilon$ -expansion [22] ( $\xi = 0.475$  and  $\lambda = 0.17$ ); and also the TF (LDA) results ( $\xi = 0.44$  and  $\lambda = 0$ ). The figure clearly shows that the simple TF predictions are not fully reliable, while the best-fit ETF functional is extremely accurate.

In Fig. 2 we report the comparison between the density profiles obtained with our best-fit ETF functional and the FNDMC results [4,5]. We have also included the SLDA results [6]. The figure shows that, near the surface, both ETF and SLDA methods are in very good agreement with the FNDMC predictions. Close to the center there are instead appreciable differences. Nevertheless, it is important to remind that in the FNDMC approach the statistical uncertainty is quite large at small distances from the center of the trap. Moreover, also SLDA values for central density depend quite a bit on the size of the BdG basis.

For the sake of completeness, in Fig. 3 we plot the zoom of the density profile  $n(r)$  near the surface for  $N = 20$ , including also the TF prediction (dot-dashed line). The figure clearly shows that the TF data are not reliable near the surface.

In our determination of  $\xi$  and  $\lambda$  we have analyzed the unitary gas with an even number  $N$  of particles. Monte Carlo calculations show a clear odd-even effect (zig-zag effect): the ground state energy of  $N$  odd particles in the isotropic harmonic trap is

$$E_N = \frac{1}{2}(E_{N-1} + E_{N+1}) + \Delta E_N , \quad (11)$$

where the splitting  $\Delta E_N$  is always positive. Dam Thanh Son has suggested [25] that, given the superfluid cloud of even particles, the extra particle is localized where the energy gap is smallest, which is near the edge of the cloud. Dam Thanh Son has also found [25] that, for fermions at unitarity, confined by a harmonic potential with frequency  $\omega$ , the odd-even splitting grows as

$$\Delta E_N = \gamma N^{1/9} \hbar \omega , \quad (12)$$

where  $\gamma$  is an unknown dimensionless constant. After a systematic investigation of the FNDMC data we find that  $\gamma = 0.856$  gives the best fit [3].

#### IV. EXTENDED SUPERFLUID HYDRODYNAMICS

Let us now analyze the effect of the gradient term (7) on the dynamics of the superfluid unitary Fermi gas. At zero temperature the low-energy collective dynamics of this

fermionic gas can be described by the equations of extended [26,27] irrotational and inviscid hydrodynamics:

$$\frac{\partial n}{\partial t} + \nabla \cdot (n\mathbf{v}) = 0 , \quad (13)$$

$$m \frac{\partial}{\partial t} \mathbf{v} + \nabla \left[ -\lambda \frac{\hbar^2}{2m} \frac{\nabla^2 \sqrt{n}}{\sqrt{n}} + \mu(n; \xi) + U(\mathbf{r}) + \frac{m}{2} v^2 \right] = 0 . \quad (14)$$

They are the simplest extension of the equations of superfluid hydrodynamics of fermions [1] where  $\lambda = 0$ .

The extended hydrodynamics equations can be written in terms of a superfluid nonlinear Schrödinger equation (NLSE), which is Galilei-invariant [3]. In fact, by introducing the complex wave function

$$\psi(\mathbf{r}, t) = \sqrt{n(\mathbf{r}, t)} e^{i\theta(\mathbf{r}, t)} , \quad (15)$$

which is normalized to the total number  $N$  of superfluid atoms, and taking into account the correct phase-velocity relationship

$$\mathbf{v}(\mathbf{r}, t) = \frac{\hbar}{2m} \nabla \theta(\mathbf{r}, t) , \quad (16)$$

where  $\theta(\mathbf{r}, t)$  is the phase of the condensate wavefunction of Cooper pairs, the equation

$$i\hbar \frac{\partial}{\partial t} \psi = \left[ -\frac{\hbar^2}{4m} \nabla^2 + 2U(\mathbf{r}) + 2\mu(|\psi|^2; \xi) + (1 - 4\lambda) \frac{\hbar^2}{4m} \frac{\nabla^2 |\psi|}{|\psi|} \right] \psi , \quad (17)$$

is strictly equivalent to the equations of extended hydrodynamics.

The extended hydrodynamics equations are the Euler-Lagrange equation of the following Lagrangian density

$$\mathcal{L} = -n \left( \dot{\theta} + \frac{\hbar^2}{8m} (\nabla \theta)^2 + U(\mathbf{r}) + \varepsilon(n; \xi) + \lambda \frac{\hbar^2}{8m} \frac{(\nabla n)^2}{n^2} \right) , \quad (18)$$

which depends on the total number density  $n(\mathbf{r}, t)$  and the phase  $\theta(\mathbf{r}, t)$  [3]. In the case  $\lambda = 0$  it is called the Popov Lagrangian of superfluid hydrodynamics [28].

Using, as previously, Eq. (15) we find that the extended Popov Lagrangian (18) is equivalent to the following one:

$$\mathcal{L} = \psi^* \left( i \frac{\hbar}{2} \frac{\partial}{\partial t} + \frac{\hbar^2}{8m} \nabla^2 - U(\mathbf{r}) - \varepsilon(|\psi|^2; \xi) \right) \psi + (1 - 4\lambda) \frac{\hbar^2}{8m} (\nabla |\psi|)^2 . \quad (19)$$

## V. SOUND VELOCITY AND COLLECTIVE MODES

From the equations of superfluid hydrodynamics one finds the dispersion relation of low-energy collective modes of the uniform ( $U(\mathbf{r}) = 0$ ) unitary Fermi gas in the form

$$\frac{\Omega}{q} = \sqrt{\frac{\xi}{3}} v_F, \quad (20)$$

where  $\Omega$  is the collective frequency,  $q$  is the wave number and

$$v_F = \sqrt{\frac{2\epsilon_F}{m}} \quad (21)$$

is the Fermi velocity of a noninteracting Fermi gas.

The equations of extended superfluid hydrodynamics (or the superfluid NLSE) give also a correcting term [3], i.e.

$$\frac{\Omega}{q} = \sqrt{\frac{\xi}{3}} v_F \sqrt{1 + \frac{3\lambda}{\xi} \left(\frac{\hbar q}{2mv_F}\right)^2}, \quad (22)$$

which depends on the ratio  $\lambda/\xi$ .

In the case of isotropic harmonic confinement, Eq. (10), we study numerically the collective modes of the unitary Fermi gas by increasing the number  $N$  of atoms. By solving the superfluid NLSE we find that the frequency  $\Omega_0$  of the monopole mode ( $l = 0$ ) and the frequency  $\Omega_1$  dipole mode ( $l = 1$ ) do not depend on  $N$ :  $\Omega_0 = 2\omega$  and  $\Omega_1 = \omega$ , as predicted by Castin [29].

We find instead that the frequencies  $\Omega_2$  and  $\Omega_3$  of quadrupole ( $l = 2$ ) and octupole ( $l = 3$ ) modes depend on  $N$  and on the choice of the gradient coefficient  $\lambda$ . The frequencies are computed by solving the time-dependent Schrödinger equation (17). We consider the initial state

$$\psi(\mathbf{r}, t = 0) = e^{i\epsilon Q_l} \psi_{gs}(\mathbf{r}), \quad (23)$$

where  $\psi_{gs}(\mathbf{r})$  is the ground-state wave function,  $\epsilon$  is a small parameter and  $Q_l$  is the operator which excites the surface mode with angular momentum  $l$  (and  $m_l = 0$ ) [17]. For the quadrupole mode one has



$$Q_2 = 2z^2 - x^2 - y^2 \quad (24)$$

while for the octupole mode the operator is

$$Q_3 = z(2z^2 - 3x^2 - 3y^2) . \quad (25)$$

Both  $Q_2$  and  $Q_3$  are expressed in cartesian coordinates [17]. In this way, a reliable value for the mode frequency can be obtained by following the real-time evolution of the system for rather short times, corresponding to few periods of oscillations at most.

In Fig. 4 we plot the quadrupole frequency  $\Omega_2$  as a function of the number  $N$  of atoms under harmonic confinement. We consider three values of the gradient coefficient  $\lambda$ . For  $\lambda = 0$  one finds  $\Omega_2 = \sqrt{2}\omega$  [1]. As shown by the figure, this is the asymptotic value one finds only for a very large  $N$  with a non-zero  $\lambda$ . Thus, we predict that finite-number effects can be detected in the unitary Fermi gas by measuring the quadrupole mode  $\Omega_2$ . This finite-number effect is stronger for surface modes with a larger angular quantum number  $l$ . This is shown in Fig. 5, where we plot the octupole mode  $\Omega_3$  as a function of  $N$ .

## VI. CONCLUSIONS

We have introduced an extended Thomas-Fermi (ETF) functional for the trapped unitary Fermi gas. By fitting FNDMC calculations we have determined the universal parameters  $\xi$  and  $\lambda$  of ETF functional. ETF functional can be used to study ground-state density profiles in a generic external potential  $U(\mathbf{r})$ . We have also introduced a time-dependent version of the ETF functional: the extended superfluid hydrodynamics (or superfluid NLSE). The superfluid NLSE can be used to investigate collective modes also for a small number of atoms. Our predictions suggest that surface effects are indeed very important for the unitary Fermi gas and that the physical observables strongly depend on them. Next-future experiments with less than one hundred degenerate Fermi atoms [30] across a Feshbach resonance can surely test our theoretical results.

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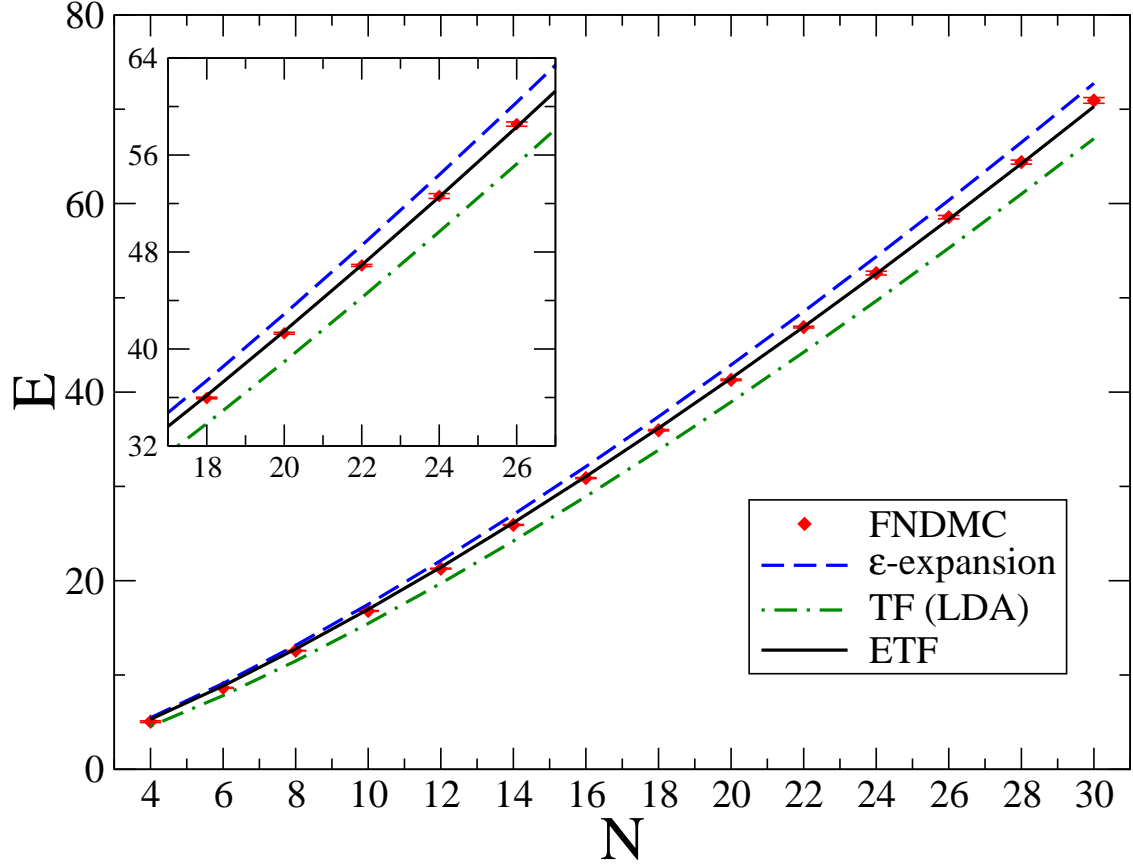
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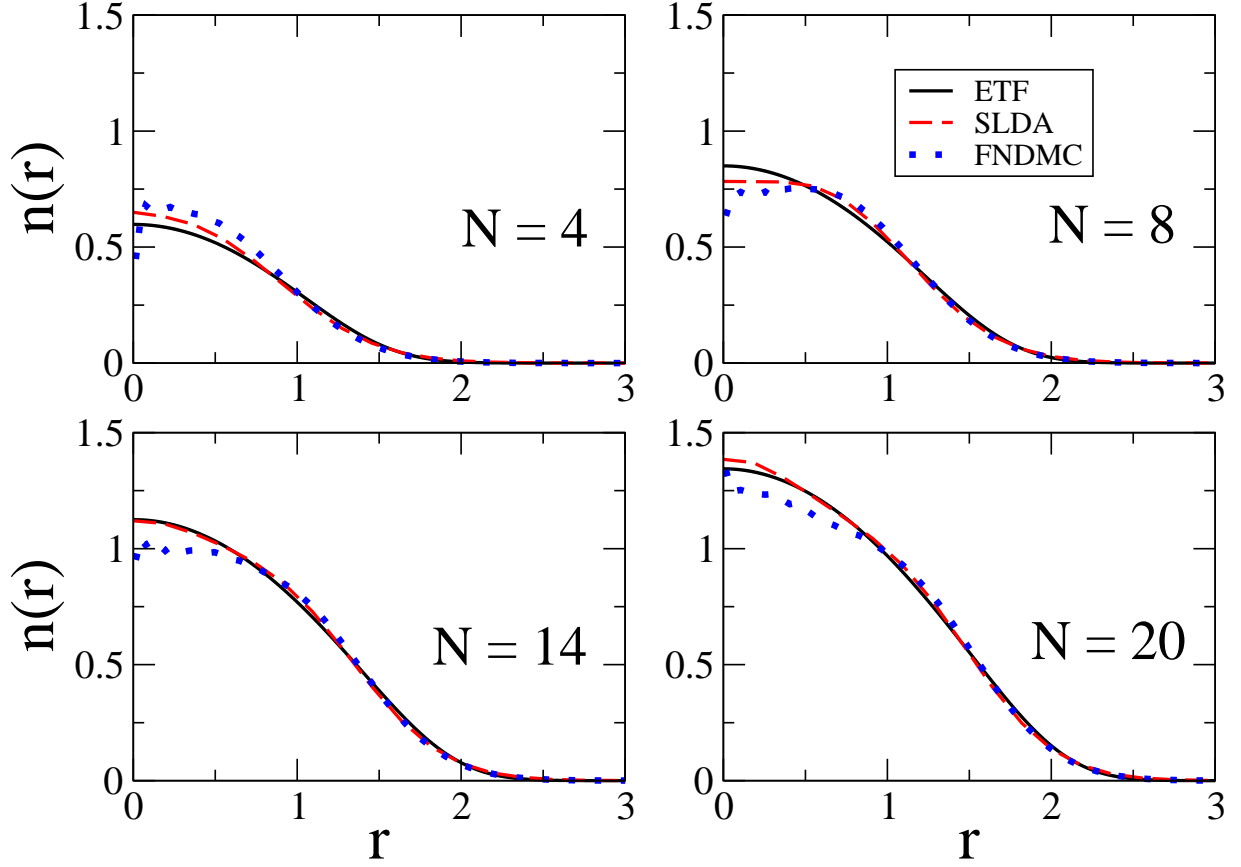
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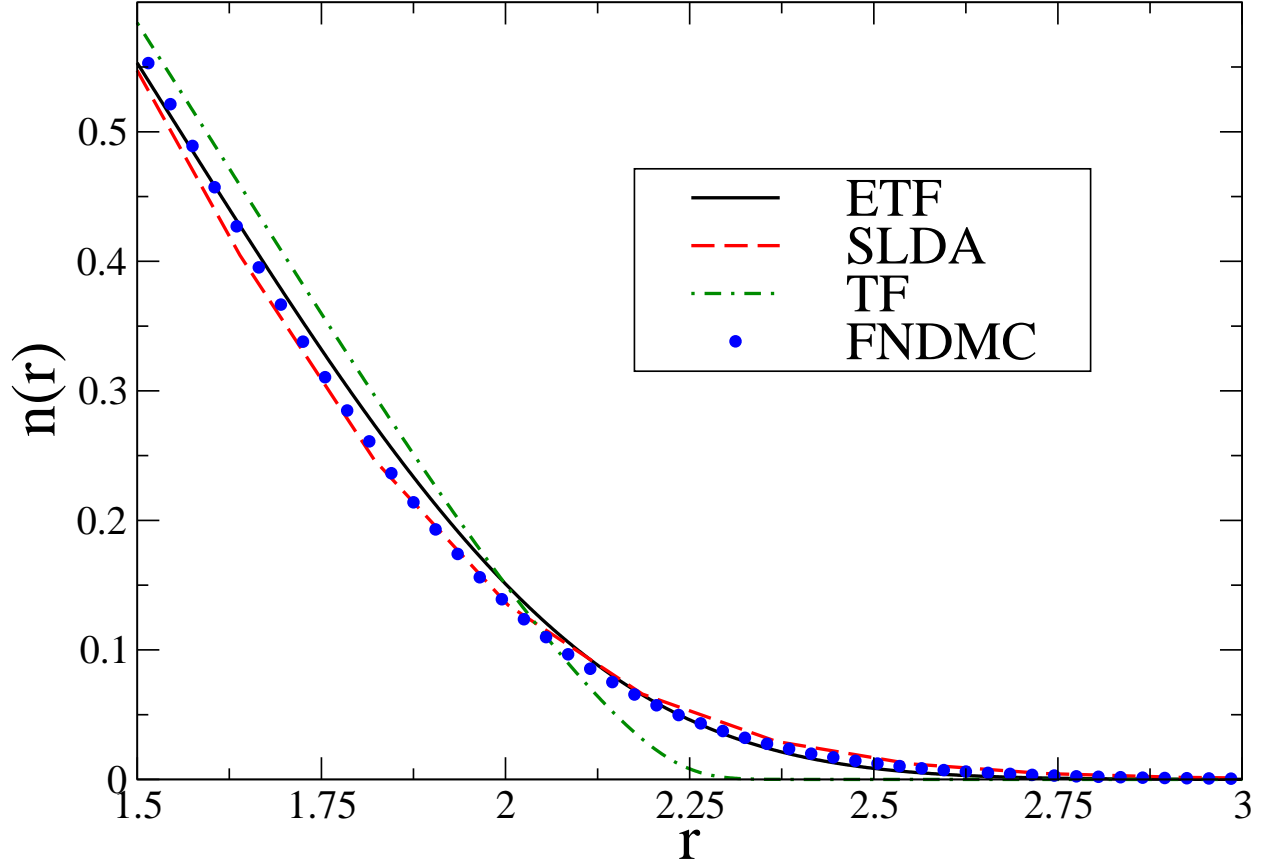
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**Fig. 1.** Ground-state energy  $E$  for the unitary Fermi gas of  $N$  atoms under harmonic confinement of frequency  $\omega$ . Symbols: FNDMC data with even  $N$  [4]; solid line: ETF results with best fit ( $\xi = 0.455$  and  $\lambda = 0.13$ ); dashed line: ETF results obtained from  $\varepsilon$ -expansion [22] ( $\xi = 0.475$  and  $\lambda = 0.17$ ); dot-dashed lines TF (LDA) results ( $\xi = 0.44$  and  $\lambda = 0$ ). Energy in units of  $\hbar\omega$ .

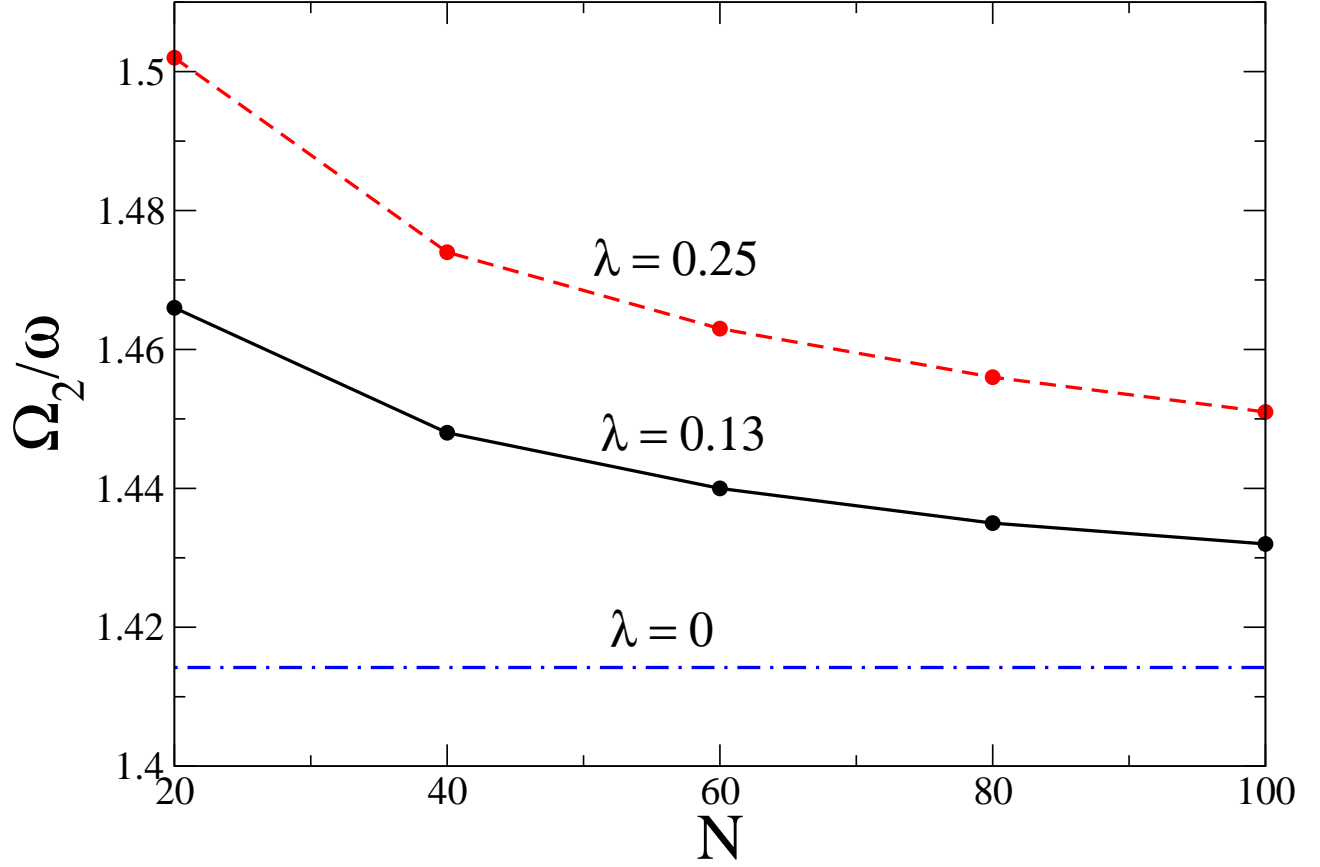


**Fig. 2.** Unitary Fermi gas under harmonic confinement of frequency  $\omega$ . Density profiles  $n(r)$  for  $N$  fermions obtained with our ETF (solid lines), SLDA [6] (dashed lines), and FNDMC [5] (filled circles). Lengths in units of  $a_H = \sqrt{\hbar/(m\omega)}$ .

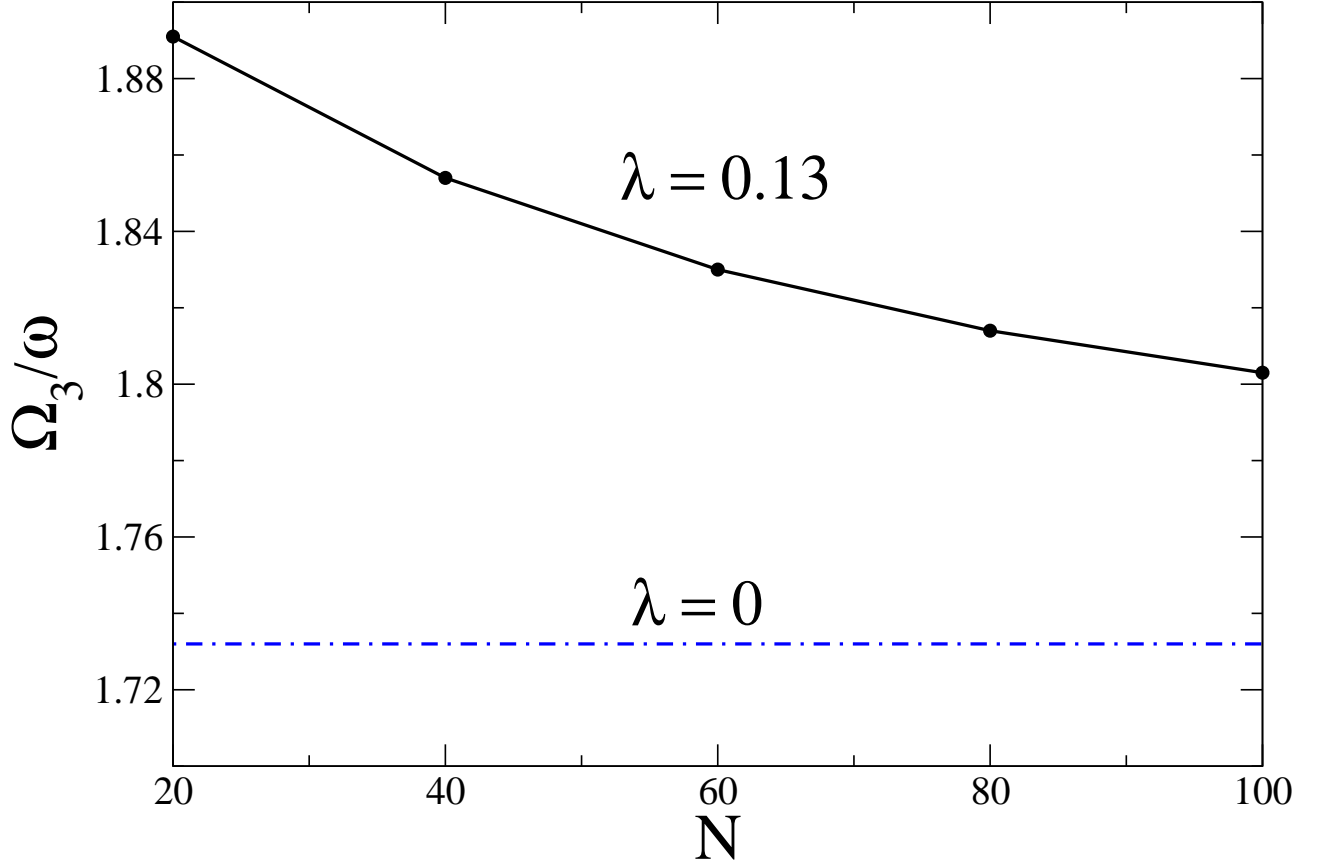


**Fig. 3.** Unitary Fermi gas with  $N = 20$  atoms under harmonic confinement of frequency  $\omega$ . Density profile  $n(r)$  near the surface obtained with our ETF (solid line), SLDA [6] (dashed line), TF (dot-dashed line), and FNDMC [5] (filled circles). Lengths in units of  $a_H = \sqrt{\hbar/(m\omega)}$ .





**Fig. 4.** Quadrupole frequency  $\Omega_2$  of the unitary Fermi gas ( $\xi = 0.455$ ) with  $N$  atoms under harmonic confinement of frequency  $\omega$ . We use three different values of the gradient coefficient  $\lambda$ . Notice that for  $\lambda = 0$  (TF limit) one finds  $\Omega_2 = \sqrt{2}\omega$ .



**Fig. 5.** Octupole frequency  $\Omega_3$  of the unitary Fermi gas ( $\xi = 0.455$ ) with  $N$  atoms under harmonic confinement of frequency  $\omega$ . We use two different values of the gradient coefficient  $\lambda$ . Notice that for  $\lambda = 0$  (TF limit) one finds  $\Omega_3 = \sqrt{3}\omega$ .

